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Comparative Study of Peat Composition by using FT-IR Spectroscopy

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Abstract. **Three nearby located mires (Svetupe, Dzelve and Eipurs Mire) were selected for this study with the aim to analyze functional groups of low moor and raised bog peat by using Fourier transform infrared spectroscopy. Functional groups of peat and their relations from two ombrotrophic and one minerotrophic mire were studied. Despite small distance between the sites, due to much diverse character of bog development, properties of the mires differ significantly. Studied peat was characterized by radiocarbon dating, loss on ignition analysis, analysis of botanical composition and decomposition degree. Infrared spectra of low moor peat help to identify the four main building structures: alcohols, aliphatic hydrocarbons, carboxylic acids (C=O band) and polysaccharides, while peat from both raised bogs shows also presence of benzene containing structures, alkenes and carboxylic acids. The results show that high decomposition degree of low moor peat simplifies infrared spectra and information of fen peat shows only most persistent structures remained in peat, while FT-IR spectroscopy provides a more detailed picture of raised bog peat.**

Keywords **– functional groups, FT-IR spectroscopy, low moor peat, raised bog peat**

I. INTRODUCTION

It has been stated that peat can serve as a good indicator of the recent and historical changes in the environment. Peat, because of its sorption abilities, gradually records fluctuations of environmental conditions. Accumulation process of peat deposits is highly regional, thus it is significant to assess every specific case individually [1]. In most cases attention is being paid on raised bogs, while low moor peat is relatively little studied. This can be explained by differences between these types of peat. Formation of raised bogs is mainly affected by atmospheric precipitations, while low moors are forced by wide range of possible contributors. Generally, it is important to reflect and isolate the natural processes in low moor peat from the effect of a wide range of possible regional geodynamical processes, pollution etc.

Nowadays fast and cheap methods are required for screening of peat chemical characteristics. Peat has a high potential in environmental purification, medicine, pharmacology, agriculture, gardening, etc. Spectroscopy is one of the appropriate research options [2], [3].

Low moors (also known as fens) are type of mire with the more than 0.4 meter thick peat soil. Vegetation receives water and nutrients from precipitation, streams and groundwater. Fens usually are of minerotrophic origin [4], [5]. In comparison with raised bogs, thickness of peat layer in low moors is relatively small; however, the area occupied by fen may be several times larger. There also exist comparative differences in peat characteristics, for instance, in the moisture and mineralization degree, decomposition degree, pH level, etc. Essential differences between peats are concentration of chemical elements and set of functional groups.

The quality of peat and range of applications largely have direct dependence upon concentration of major and trace elements presence. Ability of peat to accumulate chemical elements depends on the ability of ions to bind with characteristic functional groups. In this respect, the most significant usually are carboxyl and phenol hydroxyl groups. In the ability to accumulate elements, a noticeable role also belongs to other factors, such as water pH, content of low molecular-weight compounds, etc. However, in most cases high concentration of functional groups common to peat provides the ability to bind major and trace elements [6].

TABLE 1

COMMON FUNCTIONAL GROUPS ON FT-IR SPECTRA OF PEAT
(AFTER AIKEN, 1985)

Wavenumber, cm^{-1}	Assignment
750-880	Hydrogen-bonded OH stretching of carboxylic groups.
1040-1090	C-O stretching of alcoholic compounds, polysaccharides.
1137-1280	C-O stretching of esters, ethers and phenols.
1332-1390	Salts of carboxylic acids
1390-1400	OH deformations and C-O stretching of phenolic OH, C-H deformation of CH_3 groups.
1420-1470	Aliphatic C-H deformation.
1515	C=C stretching in benzene and/or pyridine.
1585-1640	C=O stretching of double bonds in cyclic and acyclic compounds.
1640-1725	C=O stretching of carboxylic acids.
1850-2500	Carboxylate ions.
2850-2950	Aliphatic C-H, $C-H_2$, $C-H_3$ stretching.
3030-3077	Aromatic C-H stretching.
3300-3670	Hydrogen-bonded OH groups.

Fourier transform infrared (FT-IR) spectroscopy is the method for obtaining an IR spectrum of absorption, photoconductivity, emission or Raman scattering of substances [2]. In this study it has been used to obtain infrared spectrum of the absorption of solid peat samples. FT-IR spectroscopy has several advantages against other peat research methods, such as CHNS analysis or UV/Vis spectroscopy. The general advantage is simplicity of this method. Sample preparation and analysis are not so timeconsuming and results can be obtained almost immediately. The application of FT-IR spectroscopy on peat provides data about the nature of oxygen and hydrogen containing functional groups, their structural array, relations etc. [2], [7]. However, it should be remembered that this method only indicates the presence of one or another functional group. Certain functional groups absorb IR light at characteristic frequencies (Table 1), therefore it is possible to identify chemical structures common to singular peat sample [3]. The most part of absorption zones for the functional groups common to peat are located in the so-called middle range of IR spectra at wavelength interval from 400 cm^{-1} to 4000 cm^{-1}. General absorption range can be split into three main areas: 1) the "Fingerprint region" in wavelength interval from 400 cm^{-1} to 1500 cm^{-1}; 2) absorption of double bounded groups in the range from 1500 to 2500 cm^{-1} and 3) "R-H region" in the range 2500 – 4000 cm^{-1} [2].

The goal of this study was to determine functional groups in the low moor peat from selected Svetupe Mire and to compare obtained results with the data from peat samples taken from the two raised bogs located nearby. The general idea was to find differences in the functional groups between low moor and raised bog peat by using FT-IR spectroscopy and to establish whether this method is appropriate in low moor peat research.

II. MATERIALS AND METHODS

Site Location

Single study area includes two raised bogs and low moor. All three mires are located in the central part of Latvia (Fig. 1). The Svetupe Mire is a minerotrophic low moor located in Limbazi County, North Vidzeme Biosphere Reserve. For the purpose of data comparison the two nearest ombrotrophic raised bogs in Seja district were considered: Dzelve and Eipurs Bog.

Svetupe Mire (57°32'47"N, 24°41'55"E) and Dzelve (57°13'58"N, 24°30'12"E) Bog are located in Coastal Lowland, but Eipurs (57°14'53"N, 24°37'00"E) is located in Middle Latvia Lowland. All three mires are positioned approximately 45 – 50 km NE from Riga.

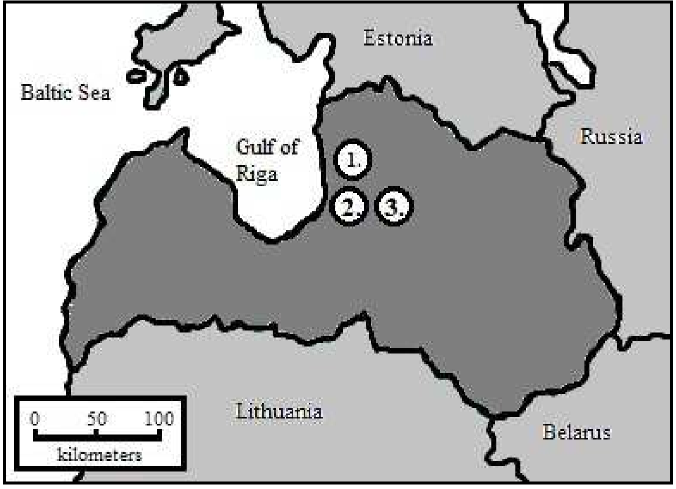

Fig.1. Location of: 1. Svetupe Mire; 2. Dzelve Bog; 3. Eipurs Bog

Sampling

Peat samples were taken from research points with "Russian" type stainless steel corer (standard peat corer). Semi-cylindrical corer with shutter was pushed into sediments, twisted and recovered to display a full and undisturbed peat profile [8–10]. In the survey the model with a sample chamber 50 cm long with inner diameter of 70 mm was used.

Sample Dating

The ^{14} Cages (yr BP) of several peat samples according to their botanical composition and deposit depth were determined by conventional radiocarbon dating [11]. In sample dating liquid scintillation counting method was used [11], [12]. As the scintillation solvent benzene was used [12]. Absolute age of peat profiles was calculated by using "Clam" v. 1.0.2 add-on for "R" v. 2.11.0 software. This program performs "classic" age-depth modelling [13]. In age modelling linear interpolation between dated levels was used and ages were calculated for each 5 cm. In calculation as calibration curve IntCal09.14C was used [14].

Determination of Botanical Composition and Decomposition Degree

The decomposition degree was determined with the help of centrifugation method according to ГОСТ 10650-72 standard [15]. Botanical composition was determined in binocular microscope at 56 to 140 times magnification by using ГОСТ 28245-89 standard [16]. The principle of this analysis is to identify the percentage of specific plant residues in the defined area, as a result all the identified plant remains constitute 100 %. Diagrams of botanical composition and decomposition degree were created with the help of "Tilia" v. 1.7.16 software.

Sample Preparation for FT-IR Analysis

Taking into account the risk of sample degradation due to oxidation, peat profiles were cut into 5 cm slices and stored at -20°C before the analysis [17]. Samples were oven-dried at 105°C for 12 hours and crushed in grinder with titanium blades [17]. Finally, the samples were sieved through the 0.25 mm sieve [3]. Homogeneous powder was transferred into sample bags and stored until performance of analysis.

Natural moisture, content of organic matter, carbonates and mineral matter was determined by parallel use of Loss on Ignition (LOI) analysis [18].

FT-IR Analysis

Samples for analysis were selected based on depth range of particular layers, botanical composition and decomposition degree of peat. IR spectra of selected peat samples were recorded by using "Perkin Elmer Spectrum BX FT-IR" spectrophotometer. To reduce errors on spectra (for instance, collection of CO_2 from the air) several background samples were prepared. Typical error usually is observable in the wavelength range from 2340 to 2300 cm^{-1} and is caused by effect of CO_2 and moisture [2], [3].

Background samples were prepared from potassium bromide (VWR International Ltd., England; KBr for infrared spectroscopy) [2], [19]. 30 mg of KBr salt were manually compressed into a pellet, through which infrared radiation was transmitted [19].

250 mg of KBr were mixed with 25 mg of sample powder and 30 mg of mixture were extracted and compressed into a pellet. The IR radiation was transmitted through the sample pellet and spectral data were recorded. IR spectra were recorded in the wavelength range from 4000 to 450 cm^{-1} with resolution of 4 cm^{-1}. The baseline correction and normalization of recorded data were performed [2], [3]. Spectral curves were visualized by using “Spekwin32” software.

III. RESULTS AND DISCUSSION

Botanical Composition, Decomposition Degree and Age of Peat

Lithology of Svetupe low moor peat is simple. Profile (Fig. 2) consists of three fen peat subtypes: wood-grass peat, wood-sedge peat and sedge peat. Major portion of the profile is characterized as sedge fen peat. In general, it is formed by such sedge species remains as *Carex lasiocarpa*, *C. elata*, *C. appropinquata*, *C. diandra* and *C. riparia*. Sedge fen peat contains the highest amount of observed *Drepanocladus* moss remains in peat profile (up to 20% of the total mass).

The highest values of decomposition degree are characteristic for the peat with wood remains (generally, pines and deciduous trees) at a depth range from 0.00 to 0.50 m (superficial peat layers). Decomposition degree in these peat layers is up to 40%. The degree of decomposition of the sedge fen peat is stable and variations by depth are within a small range from 25 to 30%.

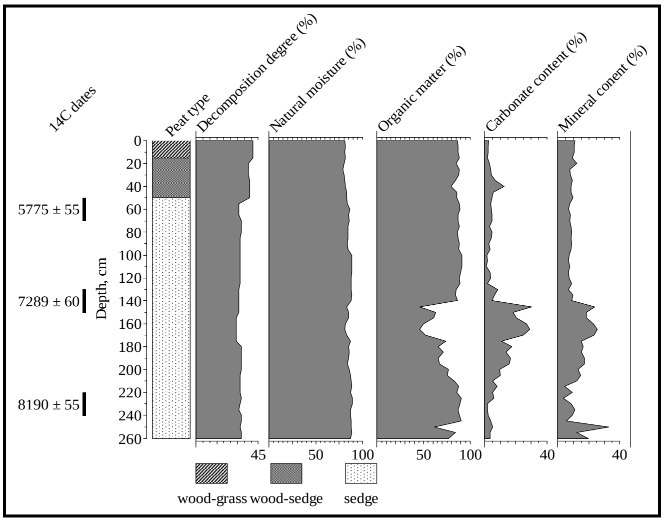

Fig.2. The structures of Svetupe low moor peat profile

Calculations show that peat accumulation in Svetupe Mire was variable. The mire developed 9500 years ago (Preboreal, early Holocene) at the approximate peat accumulation rate of 1 cm in 12 years. Peat accumulation slowed down about 8000 years ago (Atlantic, mid. Holocene), when the rate was 1 cm in every 18 years. Accumulation has slowed downed for the third time approximately 5900 years ago (Atlantic, mid. Holocene), when the rate was already 1 cm in every 130 years.

Overall, changes in peat accumulation rate are related to the botanical composition. A clear dividing line can be drawn between the sedge fen and wood-sedge fen peat, were the accumulation rate changes from 1/18 to 1/130 rapidly. In its turn, the origin of changes in accumulation rate from 1/12 to 1/18 in the sedge fen peat layer, approximately at 1.50 m, should be associated with gradual replacement of vegetation. Besides, at the depth mark of 1.50 m changes in natural moisture, content of organic matter, carbonates and minerals are observable. These parameters seem to affect some of the origin of changes in accumulation rate of peat.

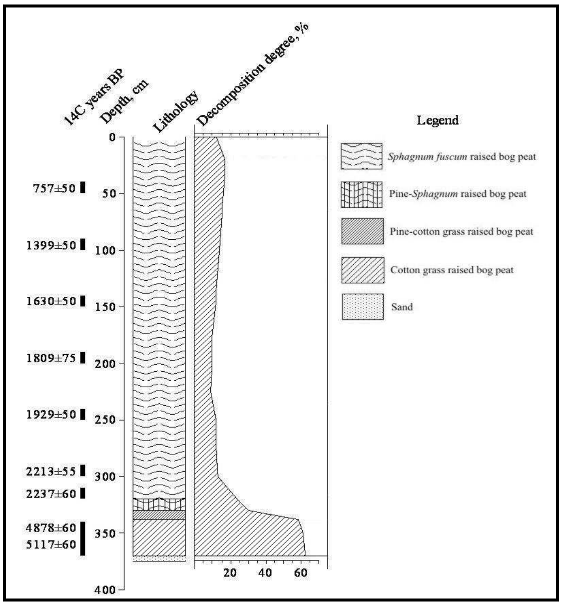

Fig.3. The structure of Dzelve raised bog peat profile

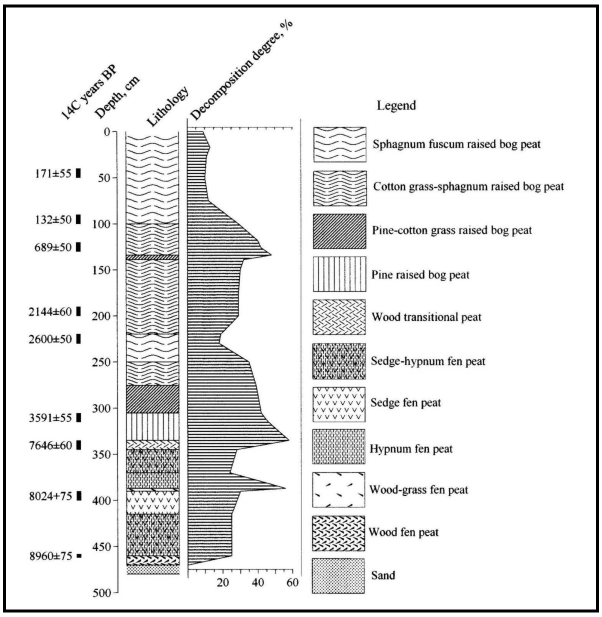

Fig.4. The structure of Eipurs raised bog peat profile

Lithology of peat from selected raised bogs is different. Dzelves Bog peat profile (3.40 m) is simple as Svetupe profile, however, peat subtypes are different. The profile (Fig. 3) consists of the four raised bog peat subtypes: *Sphagnum fuscum*, Pine-*Sphagnum*, Pine-Cotton grass and Cotton grass raised bog peat. The larger part of the profile is characterized as *Sphagnum fuscum* raised bog peat (0.00 – 3.20 m). Eipurs Bog peat profile (Fig. 4) is complicated and consists of 10 peat types (including raised bog, transitional and fen peat subtypes). In the range between 0.00 and 3.30 m raised bog peat is accumulated, within a small range from 3.30 to 3.45 m wood transitional peat, but in the remaining part fen peat is accumulated. Superficial peat layers consist of *Sphagnum fuscum*, Cotton grass-*Sphagnum*, Pine-Cotton grass and Pine raised bog peat. Bottom peat layers consist of Sedge-*Hypnum*, *Hypnum*, and wood-grass and *Equisetum* fen peat.

Decomposition degree of Dzelves peat varies from 20 to 60 %, the highest values are characteristic to pine-cotton grass and cotton grass peat in the bottom part of the profile, decomposition degree in this part of the profile reaches 60 %. In the larger part of the profile (0.00 – 3.00 m), which is characterized as *Sphagnum fuscum* raised bog peat, decomposition degree is at a stable ~20 %. In Svetupe Mire the highest values of decomposition degree are characteristic for the peat with wood remains. The situation with decomposition degree of peat in Eipurs Bog is a bit different because of varied botanical composition. However, overall, it varies within the same range from 20 to 60 % and the highest values are characteristic to peat with wood remains.

Eipurs Bog like Svetupe Mire developed in Preboreal, early Holocene, approximately 9000 years ago. Dzelves Bog is younger and developed at the end of Atlantic period, approximately 6000 years ago. It is significant to note that Eipurs Bog at the beginning developed as fen, but Dzelves Bog from the outset developed as raised bog.

Functional groups

In FT-IR analysis several peat samples from Svetupe Mire (n=35), Dzelve (n=10) and Eipurs (n=40) Bog were used. The decomposition degree, depth range and relative age of peat were taken into account in comparison among the researched sites. In the data analysis statistical significance was applied (Table 2).

TABLE 2

CRITICAL VALUES OF CORRELATION COEFFICIENT

Site	**n**	**p**	**α**
Svetupe Mire	35	0.05	0.332
Dzelve Bog	10	0.05	0.632
Eipurs Bog	40	0.05	0.310

IR spectrum covers the wavelength range from 4000 to 500 cm^{-1}. Infrared spectra of analyzed peat can be divided into several regions depending on presence of significant functional groups.

According to fundamentals of infrared spectroscopy the middle range of IR spectrum, which is comparable with peat, can be generally separated into three zones:

1.) R-H region (4000 – 2500 cm^{-1}). It is typical for O-H, N-H and C-H absorption bands.

2.) Absorption within the range from 2000 to 1500 cm^{-1} is characteristic for functional groups with double bonds. Usually these are C=O and C=C.

3.) Absorption area below 1500 cm^{-1} is called the “Fingerprint region”. In this region fluctuate functional groups with the wide non-specific absorption range. Typically in this area polysaccharide absorption bands can be observed, mostly around 1040 cm^{-1}.

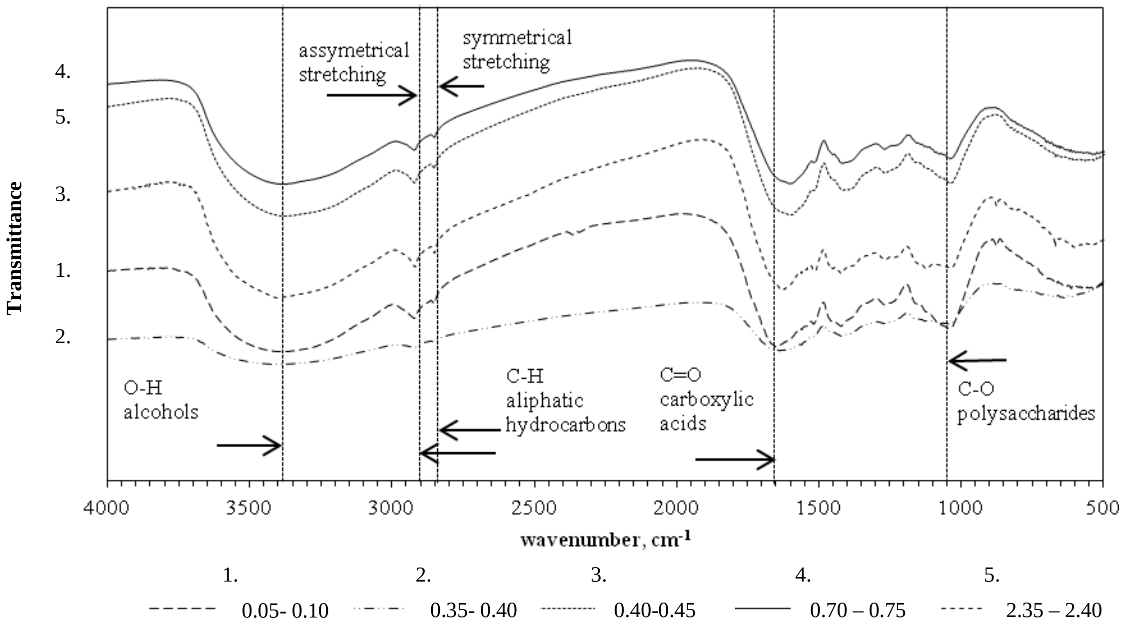

Fig.5. FT-IR spectral curves, Svetupe Mire

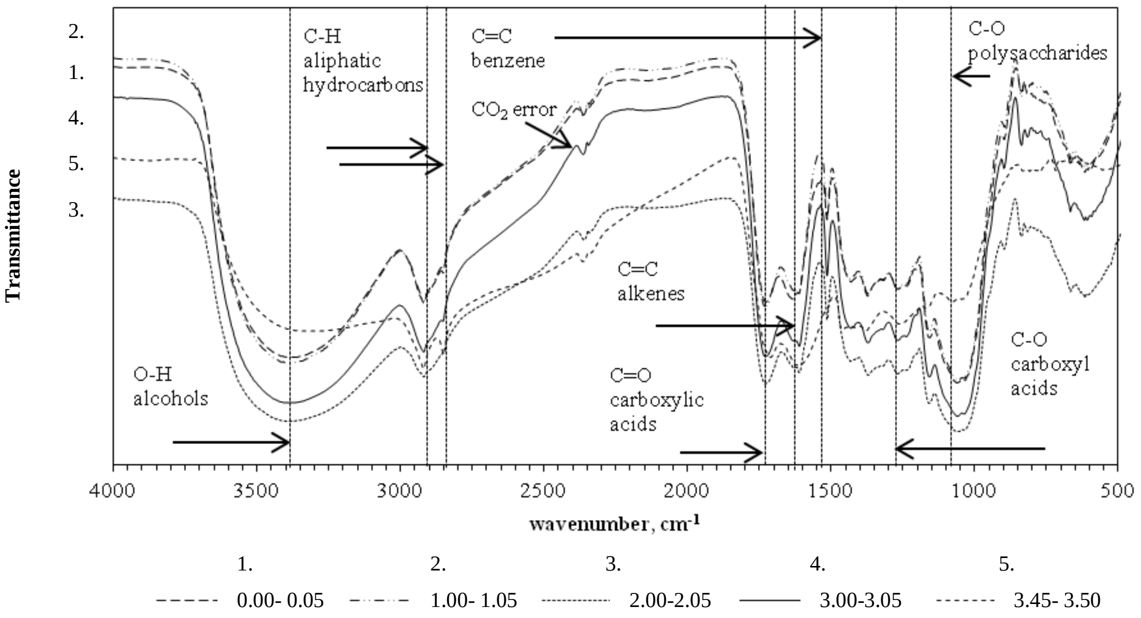

Fig.6. FT-IR spectral curves, Dzelve Bog

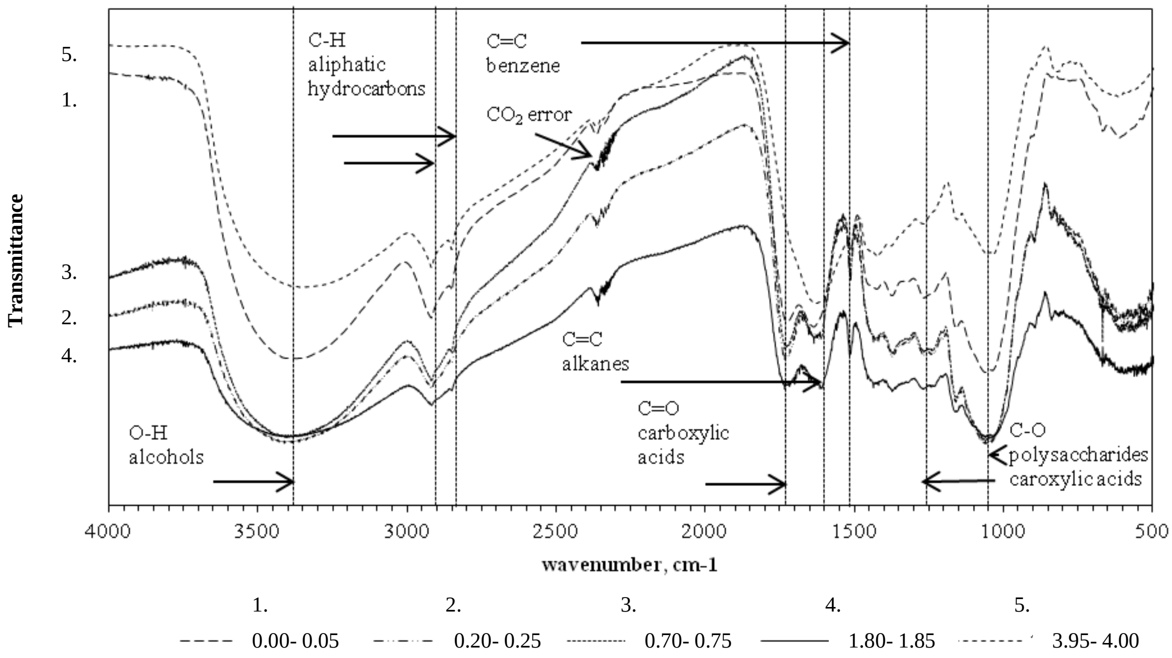

Fig.7. FT-IR spectral curves, Eipurs Bog

All recorded spectra (Table 3) are characterized by a number of absorption peaks which are pointing at different intensity that is changing with depth, degree of decomposition and is different for each mire.

In general, all collected spectra represent the same functional groups (Fig. 5-7); however, some significant differences between studied sites are also observed.

An important part of IR spectra characteristic to both raised bogs is much more complicated in comparison to low moor peat spectra. As can be noticed, the fluctuations of Dzelve and Eipurs absorption curves are not much different from Svetupe Mire; however, several absorption peaks and consequently also absorption bands significantly differs. Mainly this difference is characteristic to “Fingerprint region”. Affected are functional groups which are depending on such parameters like environmental pH and decomposition degree. Part of these functional groups, for instance, carboxylic groups (C=O), are replaced by more stable compounds because of more intensive decomposition processes. Infrared spectra of the given low moor peat reflect the four main functional groups: alcohols, aliphatic hydrocarbons, carboxylic acids (C=O band) and polysaccharides, while peat from both raised bogs shows supplement of well expressed benzenes, alkenes and carboxylic acids (with C-O band). Results show that high the decomposition degree of low moor peat simplifies infrared spectra and information of fen peat remains only in most persistent functional groups, thus FT-IR spectroscopy provides a more detailed picture of the raised bog peat.

In all cases, much more pronounced absorption bands represent a higher concentration of characteristic compounds, therefore and thus concentration of functional groups. For example, more pronounced C-H absorption bands describe higher concentration of aliphatic compounds (methyl and/or methylene groups) in a specific peat sample and this, in its turn, points to a higher decomposition degree. By following this fact it is possible to trace relative differences in absorption bands of the two paired functional groups. Unfortunately, this relation works only with the given raised bog peat samples, but not with low moor peat; the reason might be high and relatively stable degree of decomposition. Statistical data analysis shows no significant correlation among any of the functional groups in fen peat.

TABLE 3

THE REPRESENTATIVE PEAT SAMPLES USED IN FT-IR ANALYSIS

Mire	Depth, cm	Peat type	Decomposition degree, %
Svetupe	5 – 10	wood-grass, fen	41
	35 – 40	wood-sedge, fen	39
	40 – 45	wood-sedge, fen	39
	70 – 75	sedge, fen	33
	235 – 240	Sedge, fen	32
Dzelve	0 – 5	sphagnum, bog	10
	100 – 105	sphagnum, bog	11
	200 – 205	sphagnum, bog	9
	300 – 305	sphagnum, bog	13
	345 – 350	pine-cotton grass, bog	58
Eipurs	0 – 5	sphagnum, bog	10
	20 – 25	sphagnum, bog	15
	70 – 75	sphagnum, bog	13
	180 – 185	sphagnum-cotton grass, bog	28
	395 - 400	pine-cotton grass, fen	30

Absorption bands in the spectral region at wavelengths from 3700 to 3000 cm^{-1} were very broad, and at the same time the least variable (Fig. 5-7) depending on the changes in peat characteristics, depth or age. Absorbance in this region is determined by the presence of -OH groups and alcohols in studied peat. Broad absorption band at approximately 3400 cm^{-1} in all three mires applies to O-H stretching of hydrogen bonded O-H groups. According to recordings of spectra from Svetupe fen peat O-H absorption band gradually becomes a little curved. This deflection is more pronounced in the bottom peat layers, which are characterized as sedge fen peat. Very specific indeed is the sample from Svetupe is “0.35-0.40 m”: spectral curve of this sample is almost flat and it refers to wood-sedge fen peat. Some mild fluctuations in the range of absorption centre are observed. Stretching of O-H bonds in the samples from all examined sites are similar, and there are no significant differences registered between fen and raised bog peat. All peat samples were oven-dried at 105°C for 24 hours; however, considerable amount of water may remain in adsorbed form, and it is presumed that flatter O-H stretching is affected by such water content (for instance, in the “0.35-0.40 m” sample).

The absorption at the range from 3000 to 2800 cm^{-1} shows presence of alkanes. Twin peaks at about 2920 and 2850 cm^{-1} are found because of symmetrical and asymmetrical stretching of aliphatic C-H. All spectral curves of Svetupe fen peat have both peaks within this absorption range. The first peak at 2920 cm^{-1} features asymmetrical stretching of C-H bonds; the second peak shows symmetrical stretching. Absorption of aliphatic hydrocarbons is similar in all recorded spectra. Locations of both absorption peaks show presence of methyl group of aliphatic hydrocarbons in the studied peat samples.

Recordings of fen peat spectra show only one significant peak in the range from 2000 to 1500 cm^{-1}. This absorption zone might indicate two different functional classes common to peat. The concavity can be made by stretching of C=C bonds in alkanes (aliphatic hydrocarbons) and by stretching of C=O bonds in carboxylic acids as well. It is significant to notice that C=C absorption band does not correspond in any of fen peat samples, which leads to the conclusion that C=C bonds are totally collapsed. This situation is characteristic also to several peat samples from Dzelve and Eipurs Bog; here this is common to deeper peat layers with higher decomposition degree. It can be assumed that C=C alkenes and benzenes are dependent on decomposition degree and depth range of peat sample. Their concentration decreases with the increase of decomposition degree of peat.

Wavelength range from 1450 to 1355 cm^{-1} points to stretching of C-O-H bonds in carboxylic acids. FT-IR recordings show that presence of carboxylic acids in fen peat is more characteristic and more expressed than in bog peat. The concavity within the range from 1290 to 1235 cm^{-1} also indicates presence of carboxylic acids in fen peat, this zone represents stretching of C-O bonds in carboxylic groups and/or ethers.

The last highlighted absorption zones are located in the wavelength range from 1170 to 990 cm^{-1}, which represents presence of polysaccharides in the studied peat. This zone shows stretching of C-O bonds. A small peak at about 1156 cm^{-1}, is probably due to O–H stretching of alcoholic groups. Fluctuations in the spectra below 650 cm^{-1} points to COOH deformation; however this is more intensive in the spectra of both bogs, and less in fen peat.

Relations between functional groups

In addition to identifying the same functional groups, their relations were also calculated. Overall relations between O-H and C-H, C-O, C=C and C=O were calculated C-H/O-H, C-O/O-H, C=C/O-H and C=O/O-H). As it is seen, a number of these absorption bands correspond to many chemical compounds (see pictures above). In this case C-H characterize aliphatic hydrocarbons (asymmetrical stretching, wavenumber at ~2930 cm^{-1}); C=O bond describes carboxylic acids (wavenumber ~1625 cm^{-1}); C=C bond indicate alkenes (wavenumber ~1615 cm^{-1}) and C-O bond features polysaccharides (wavenumber ~1010 cm^{-1}).

In each case O-H absorption bands were selected as the basis. The intensity values of absorption bands were attributed to alcohols. Alcohols were selected, because in theory and also in practice their values do not change rapidly and significantly with depth or age of peat sample, thus it is possible to track changes in other absorption bands and in relations with them.

Infrared spectra of low moor peat samples reflect four characteristic functional groups. O-H, C-H, C=O and C-O groups. O-H group is relatively stable in full peat profile and is not affected by decomposition, however, height of absorption peaks and absorption interval are slightly affected by the depth range. In each case O-H absorption bands were selected as the basis. The intensity values of absorption bands were attributed to alcohols, decomposition degree and depth. For statistical analysis data from 35 peat samples was used. According to statistical significance at n=35 and p=0.05 alpha value is 0.332. Results show that there are no significant correlations between decomposition degree and any of the functional groups. According to statistics it is not significant, but the movement of absorption centres and intensity of absorption peaks are also observable depending on decomposition and depth of peat (Fig. 8). Another important fact is that no significant correlations between O-H and other functional groups exist, which means that groups in the given low moor peat are virtually independent from one another.

In examples with Dzelve and Eipurs raised bog peats the relation of C=O/O-H is affected by decomposition degree. In addition, this relation becomes smaller with the increase of decomposition degree. This means that carboxylic acids disintegrate as a result of decomposition and are replaced with more stable and resistant compounds. The main conclusion is that C=O groups are non-persistent to decomposition. Another significant observation is that there are also differences in the relation of C=O/O-H and depth. It can be noticed that in raised peat samples, which correspond to deeper peat layers no C=O absorption bands are present at all – carboxylic acids might have totally disintegrated. In the example with Svetupe fen peat the relation of C=O/O-H looks a bit different. First of all C=O absorption bands are represented in all peat samples. Second, intensity of peak of carboxylic acids is increasing with depth but also it is affected by decomposition degree like it is in raised bog peat samples. Only in this case decomposition degree is decreasing by depth. Decomposition degree in fens is increasing gradually and because of gradually decreasing of groundwater influence in it bacterial activity can take place more intensively.

In peat samples of Dzelve and Eipurs Bog the relation of C-H/O-H is increasing with depth as well as with the degree of decomposition. C-H absorption band describes aliphatic hydrocarbons and presence of methyl and/or methylene groups in peat. Development of these groups is characteristic to decomposition process, thus their higher concentration is represented in better decomposed peat. In the samples from both bogs more pronounced is the asymmetrical stretching of C-H, which is characteristic to wavenumber ~2920 cm^{-1}. The relation of C-H/O-H in peat samples from Svetupe Mire is decreasing with depth but increasing with the increase of decomposition degree. Because of higher decomposition degree of fen peat C-H absorption band is also more pronounced in comparison to the selected raised bog peat samples. Unlike Dzelve and Eipurs raised bog peat samples in Svetupe fen peat symmetrical stretching of C-H at the wavenumber of 2850 cm^{-1} is more pronounced.

Analysis of raised bog peat samples shows that relation of C=C/O-H absorption bands are increasing with depth and degree of decomposition. It indicates an increase of concentration of alkenes in peat. Spectral analysis, in its turn, showed that there are no C=C absorption bands in any fen peat sample.

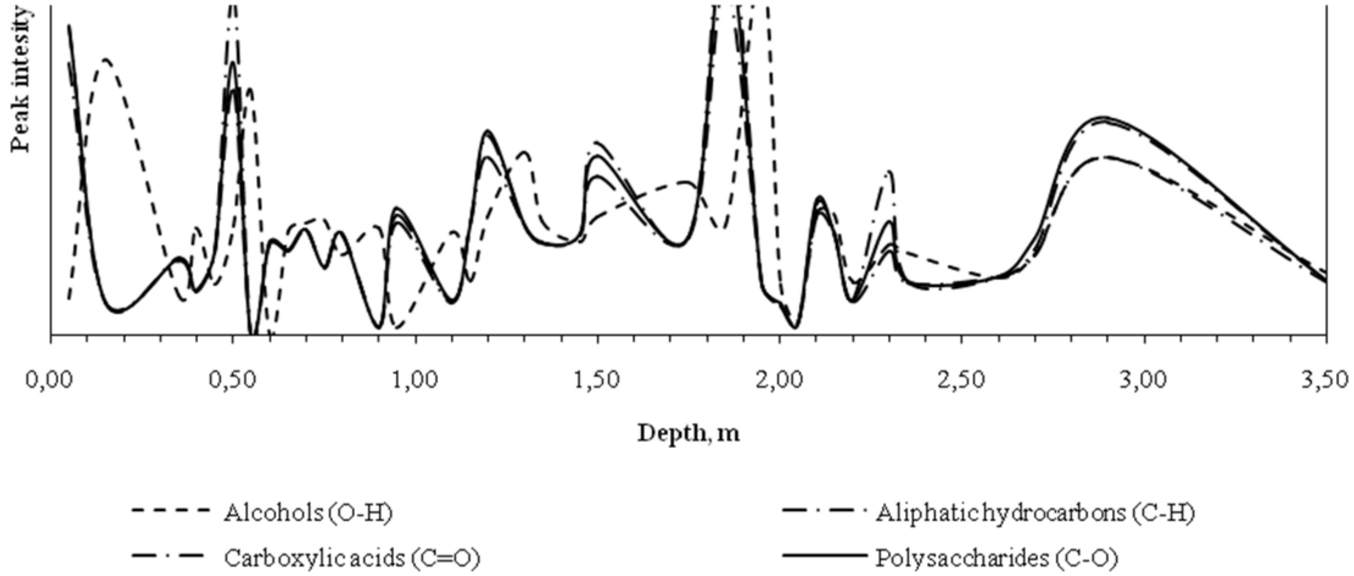

Fig.8. Absorption peak intensity fluctuations by depth, Svetupe Mire

The relation of C-O/O-H the absorption bands characterize fluctuations in concentration of polysaccharides in peat profile. In raised bog peat the concentration of polysaccharides is decreasing with depth and with the increase of decomposition degree. At the same time, the relation of these absorption bands in Svetupe fen peat is increasing with depth, but is also affected by decomposition degree – because of that concentration of polysaccharides is lower in comparison to raised bog peat.

IV. CONCLUSIONS

All FT-IR spectra are similar, because the dominant functional groups in both fens and raised bogs are similar. Overall, four absorption bands were identified in Svetupe fen peat and six in Eipurs and Dzelve raised bog peat. The number of absorption peaks points to a gradual change in relative concentrations of certain functional groups common to peat. Important absorption maximums lie within the range from 4000 to 3000 cm^{-1}, which is characteristic for hydroxyl groups and there are some differences in the intensity with respect to other groups. Despite the fact that all peat samples were oven-dried at 105°C for 24 hours, a considerable amount of water may still remained in them in the adsorbed form, and presumably that flatter stretching of O-H and other bonds are affected by this water. The main difference in the relations among absorption bands are determined by sample depth and decomposition degree of peat. Owing to higher decomposition degree of fen peat part of the functional groups, which are common to “fingerprint region”, are collapsed and replaced with more stable and resistant compounds. Because of high decomposition degree of fen peat the C=C bonded alkenes and benzenes are fully replaced, while they are present in the raised bog peat with significantly lower decomposition degree. C=O groups are non-persistent to decomposition. In case of raised bogs decomposition degree is increasing with depth, while in fens it is decreasing and all functional groups, which are subordinate to that in comparison are positioned upside down.

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Jānis Krūmiņš, Māris Kļaviņš, Valdis Segliņš, Enn Kaup. Kūdras funkcionālo grupu salīdzinošā analīze, izmantojot FT-IR metodi

Šī pētījuma ietvaros tika izvēlēti trīs relatīvi netālu izvietoti purvi (Svētupes, Dzelves un Eipura purvs). Darba mērķis bija, izmantojot Furjē infrasarkanās spektroskopijas metodi, izanalizēt kūdrā esošās funkcionālās grupas. Galvenā pētījuma ideja bija atrast funkcionālo grupu sadalījuma un attiecību atšķirības zemā un augstā tipa kūdras nogulumu paraugos. Noņemto kūdras profilu raksturošanai papildus tika izmantota radioaktīvā oglekļa datēšana, karsēšanas zudumu analīze, kā arī botāniskā sastāva un sadalīšanās pakāpes analīze. Zemā tipa kūdras paraugos infrasarkanais spektrs norāda uz piecām skaidri izteiktām funkcionālajām grupām – alkoholiem, alifātiskajiem ogļūdeņražiem, karboksilskābēm, fenoliem un polisaharīdiem. Augstā tipa kūdras paraugu spektros papildus izdalās arī benzēni un alkēni. Rezultāti norāda, ka alkēni zemā tipa kūdrā, salīdzinot ar augstā tipa kūdru, ir mazāk izteikti, tomēr alifātisko C-H saišu simetriskā izstiepšanās ar absorbcijas centru pie 2850 cm^{-1} ir vairāk raksturīga tieši zemā tipa kūdras paraugu spektriem. C-O izstiepšanās polisaharīdos ar absorbcijas centru pie ~1050 cm^{-1} sakarā ar augstāko sadalīšanās pakāpi ir izteiktāka zemā tipa kūdrā, un polisaharīdu daudzums šeit ir būtiski atkarīgs no iegulas dziļuma un kūdras vecuma. Saistībā ar zemā tipa kūdras pretēji vērsto sadalīšanās pakāpi (samazinās virzienā uz leju) visas tai pakārtotās funkcionālās grupas lielākā daudzumā ir profila augšējos slāņos salīdzinājumā ar augstā tipa kūdru, kur to vairāk ir profila apakšējos slāņos. Kopumā gan zemā tipa, gan arī augstā tipa kūdras IS spektri ir līdzīgi, tāpēc ka dominējošās funkcionālās grupas ir tās pašas. Tomēr mainās šo grupu intensitātes un savstarpējās attiecības saistībā ar atšķirīgām kūdru sadalīšanās pakāpēm, pH vērtībām u.c. parametriem. Furjē infrasarkanā spektroskopija ir lietderīga kūdras izpētes metode, tomēr jāņem vērā, ka šī ir tikai informatīva metode un ticamu rezultātu iegūšanai ir svarīgi izvēlēties arī citas izpētes metodes.

Янис Круминьш, Марис Клявиньш, Валдис Сеглиньш, Энн Кауп. Сравнительный анализ функциональных групп торфа с использованием ИК-Фурье спектроскопии.

В рамках этого исследования были выбраны 3 относительно близко расположенные друг к другу болота – Светупе, Дзелвес и Ейпурс. Цель работы, - используя метод инфракрасной спектроскопии Фурье, проанализировать существующие в отложениях торфа функциональные группы и их отличия в зависимости залегания торфа верхового или низинного типа болот. В образцах профилей дополнительно определены датирование возраста торфа (используя радиоуглеродный метод), потери при прокаливании, а также, ботанический состав и степень его разложения. В образцах торфа болот низинного типа инфракрасный спектр указывает на пять явно выраженных групп – алканы, алифатические углеводороды, карбоксильные группы, фенолы и полисахариды. В торфе верховых болот спектры дополнительно выделяют алкены. Результаты показывают, что алкены в торфе низинного типа выражены меньше чем в образцах верхового типа, однако, алифатическое C - H звено симметрично растянутое с центром абсорбции около 2850 см$^{-1}$ больше характерно для спектров образцов торфа низинного типа. Раскладка C - O полисахаридов с центром абсорбции около 1050 см$^{-1}$ в связи с высокой степенью разложения характерна для торфа низинного типа и количество полисахаридов напрямую связано с глубиной залегания и возрастом образца. Связанная с низинным типом торфа противоположно направленная степенью разложения, все те подчиненные функциональные группы в большинстве наблюдаются в верхних слоях по сравнению с верховым типом торфа, в котором этих групп как раз больше наблюдается в нижних слоях образцов. В общем, как для образцов торфа низинного типа, так и торфа верховых болот ИК спектры сходны, потому как доминирующие функциональные группы те же самые. Однако, интенсивность изменений эти групп и взаимоотношения связанны с различиями степени разложения торфа, величиной pH и др. параметрами. Инфракрасная спектроскопия Фурье весьма полезный метод изучения характеристик торфа, однако, надо иметь ввиду, что это только информативный метод и более достоверные результаты могут быть получены с привлечением и других аналитических методов.